

Positron covalent bonding

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Some of us recently reported on the energy stability of a fundamentally different type of positronic molecule [1], formed by two otherwise repelling hydride anions and one positron, $e^+[\text{H}^-\text{H}^-]$. We now present a computational study on homo- and heteronuclear $e^+[\text{X}^-\text{Y}^-]$ compounds formed by two halide anions ($\text{X}^-, \text{Y}^- = \text{F}^-, \text{Cl}^-, \text{Br}^-$) and one positron. Our results indicate the formation of energetically stable positronic molecules in all cases. The analysis of the electronic and positronic densities point out that the formation of positronic covalent bonds underlie the stabilization of the otherwise repelling dihalides. In several aspects, the positronic dihalides are similar to the purely electronic analogs, $e^-[\text{A}^+\text{B}^+]$ (AB^+), molecular cations with isoelectronic atomic cores ($\text{A}^+, \text{B}^+ = \text{Na}^+, \text{K}^+, \text{Rb}^+$) bound by one electron. Although, the vibrational parameters are always comparable, as well as the ground-state positron and spin densities at the internuclear region and the bond energies the data shows that positron bonding is somewhat stronger than regular electronic bonding in di-cation systems.

[1] J. Charry, M. T. d. N. Varella and A. Reyes, *Angew. Chemie Int. Ed.* **2018** 57, 8859